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Determination of Intermolecular Interactions in Polar and Non-polar Organic Molecules by Optical (Refractive Index) Method

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ABSTRACT

Refractive indices and densities have been experimentally determined for the binary mixtures of Toluene -Benzene, Ethanol-Benzene, Toluene-Ethanol and Water-Ethanol systems at room temperature over the entire range of mole fraction. The experimental values of refractive index and densities are utilized to calculate excess refractive indices, molar refractions, excess molar refractions, excess molar volume and calculated molar refractions. Results obtained indicate that the optical method is more accurate over the volumetric method. A strong association was observed in polar-polar solvent system and non-polar - non-polar systems.

Keywords: Refractive index, Excess refractive indices, Molar refractions, Excess molar volume, Optical, Volumetric, Polar, Non-polar.

INTRODUCTION

Refractive index measurement is an essential part of the thermodynamic studies of liquid-liquid mixtures, used to explain intermolecular interactions present amongst the mixing components[1]. It is also essential for the determination of composition of

binary liquid mixtures[2]. Complex formation in liquid mixtures has been extensively studied using optical and ultrasonic technique by many workers[3]. The formation of hydrogen bond in solutions and its effect on the physical properties of the mixtures have gained much attention[4,5]. In particular, relevance does the nature of interactions of solvent with solute species, the behavior of solvent medium in presence of other species affect the structural properties of both solvent and solute molecules. Therefore, excess properties of solutions have proven to be very useful tool in elucidating the structural interactions occurring in solution and to study solute-solvent interactions[6].

In our present study, we select polar molecules as water and ethanol, and non polar molecules as benzene and toluene. These molecules are very important in various fields of chemical sciences like, solvent as reaction medium, in solvent extraction processes, in chromatographic techniques and in drug formulation. In our present research work, refractive indices and densities of binary liquid-liquid mixtures of Toluene -Benzene, Ethanol-Benzene, Toluene-Ethanol and Water-Ethanol at room temperature over the entire range of mole fraction have been determined. Along with refractive index and density, deviation in refractive indices, molar refractions, deviation in molar refractions and excess molar volume have been calculated[7-10] and correlation have been established in terms of intermolecular interactions present amongst the components of mixtures.

MATERIALS AND METHODS

All the chemicals used were of A. R. grades. The chemicals were purified by distillation and only middle fraction was used. Solutions were prepared by mole fraction method. The weighing was done by using electronic balance with precision of ± 0.1 mg. Refractive indices (at 589.5 nm sodium line) were measured by using Abbe's Refractometer with constant temperature thermostat with precision of ±0.001 and values provided here are the mean values from three independent readings for each sample. Densities were measured using specific gravity bottle at constant temperature (298.15K).

RESULTS AND DISCUSSION

The change in refractive indices on mixing (Δn_D), excess molar volumes (V^E), excess molar refraction ($R^E m$), calculated molar refraction, also densities , refractive indices of pure liquids and entire range of mixtures of liquid listed in table no. 1, 2, 3, 4 and 5.

The values of), excess refractive indices (Δn_D), excess molar volumes (V^E), excess molar refraction ($R^E m$) for binary mixtures of toluene-benzene, ethanol-benzene toluene-ethanol and water-ethanol were calculated from data of the density ,refractive index and molar mass using following equations.

$$\Delta n = n_D-(x_1 n_{D1}+x_2 n_{D2}) \quad (1)$$

In this equation, x_1, x_2 are mole fractions. n_D, n_{D1}, n_{D2} are the refractive index of mixture, pure components 1 and2 respectively (Ku et al.,2008).

$$V^E = [(x_1M_1+x_2M_2)/p- (x_1M_1/p_1+x_2M_2)/p_2)] \quad (2)$$

In this equation x_1,x_2 are mole fractions.M_1,M_2 are molar masses, p , p_1 and

p_2 are the densities of mixtures, pure components of 1 and 2 respectively (Li *et al*., 2007).

$$R^E_M = R_M - (x_1R_{M1}+x_2R_{M2}) \quad (3)$$

In this equation x_1,x_2 are mole fractions. R_M molar refraction of binary mixtures, R_{M1} and R_{M2} are molar refractions of pure components.

Table no. : 1 - For Pure Liquids

Compound	Molar mass	Density p (g/cm^3)	Refractive index(n)	Molar refraction (cm^3/moL)	Calculated molar refraction (cm^3/moL)
Benzene	78.0	0.879	1.499	26.05495	26.289
Toluene	92.14	0.8736	1.497	30.86323	30.78
Ethanol	46.08	0.8873	1.41748	13.07307	12.961
Water	18.0	0.9954	1.3426	3.81665	3.574

Table no. : 2- Toluene-Benzene System

x_1	x_2	Density p (g/cm)	Refractive index (n)	Excesses refractive index	Molar refraction (Rm) (cm^3/moL)	Excesses molar volume (V^E) (cm^3/moL)	Rm calculated (cm3/moL)	Excesses molar refractionR^Em (cm^3/moL)
0.9	0.1	0.8168	1.45564	-0.04156	30.17329	-11.3227	30.3309	-0.20911
0.8	0.2	0.8189	1.46066	-0.02234	29.9082	-9.36278	29.8818	0.00663
0.7	0.3	0.8195	1.46268	-0.02232	29.52418	-7.39929	29.4327	0.10344
0.6	0.4	0.8200	1.46369	-0.02331	29.08606	-5.44507	28.9836	0.14615
0.5	0.5	0.8215	1.46972	-0.01928	28.87715	-3.56027	28.5345	0.41806
0.4	0.6	0.8271	1.47274	-0.01826	28.36037	-1.99172	28.0854	0.38211
0.3	0.7	0.8493	1.48076	-0.01224	27.5459	-1.82729	27.6363	0.04847
0.2	0.8	0.8596	1.48879	-0.00621	27.12841	-1.06418	27.1872	0.11181
0.1	0.9	0.8637	1.49682	-0.00018	26.89716	0.08158	26.7381	0.36139

Table no. : 3 - Ethanol-Benzene System

x_1	x_2	Density p (g/cm)	Refractive index (n)	Excesses refractive index	Molar refraction (Rm) (cm^3/moL)	Excesses molar volume(V^E) (cm^3/moL)	Rm calculated (cm3/moL)	Excesses molar refractionR^Em (cm^3/moL)
0.9	0.1	0.8051	1.45362	0.02799	16.56113	-4.45303	14.2938	2.18988
0.8	0.2	0.8145	1.45665	0.02287	17.53102	-3.27685	15.6266	1.86076
0.7	0.3	0.8253	1.45766	0.01572	18.38929	-2.36482	16.9594	1.42166
0.6	0.4	0.8360	1.45868	0.00859	19.23199	-1.686	18.2922	0.96617
0.5	0.5	0.8468	1.45968	0.00144	20.05419	-1.23928	19.625	0.49018
0.4	0.6	0.8577	1.46772	0.00133	21.13097	-1.01892	20.9578	0.26878
0.3	0.7	0.8687	1.47273	0.00181	22.08531	-1.01953	22.2906	-0.07507
0.2	0.8	0.8793	1.48868	0.00598	23.49355	-1.19479	23.6234	0.03498
0.1	0.9	0.8899	1.49282	0.00197	24.42297	3.62927	24.9562	-0.33379

Table no. : 4 - Toluene-Ethanol System

x_1	x_2	Density p (g/cm)	Refractive index (n)	Excesses refractive index	Molar refraction (Rm) (cm^3/moL)	Excesses molar volume(V^E) (cm^3/moL)	Rm calculated (cm3/moL)	Excesses molar refractionR^Em (cm^3/moL)
0.9	0.1	0.8762	1.49682	0.00804	29.22441	-11.3227	28.9981	0.1402
0.8	0.2	0.8642	1.48779	0.00723	27.63685	-9.36278	27.2162	0.33166
0.7	0.3	0.8571	1.47572	0.00339	25.76101	-7.39929	25.4343	0.23483
0.6	0.4	0.8428	1.46570	0.000159	24.21118	-5.44507	23.6524	0.46402
0.5	0.5	0.8371	1.46506	0.000917	22.82594	-3.56027	21.8705	0.85779
0.4	0.6	0.8247	1.45506	0.00739	21.22362	-1.99172	20.0886	1.03449
0.3	0.7	0.8174	1.44059	0.00114	19.33515	-1.82729	18.3067	0.92504
0.2	0.8	0.8046	1.43545	0.00423	17.9481	-1.06418	16.5248	1.317
0.1	0.9	0.7943	1.42647	0.00347	16.36602	0.08158	14.7429	1.51394

Table no. : 5 - Water-Ethanol System

x_1	x_2	Density p (g/cm)	Refractive index (n)	Excesses refractive index	Molar refraction (Rm) (cm^3/moL)	Excesses molar volume(V^E) (cm^3/moL)	Rm calculated (cm3/moL)	Excesses molar refraction R^Em (cm^3/moL)
0.9	0.1	0.9640	1.35515	0.00533	4.70605	-0.48806	4.7212	-0.03624
0.8	0.2	0.9495	1.35716	-0.00189	5.45028	-0.74695	5.5794	-0.21766
0.7	0.3	0.9392	1.35817	-0.0091	6.18089	-0.91917	6.3901	-0.4129
0.6	0.4	0.9303	1.36018	-0.01632	6.93792	-1.01008	7.3288	-0.5813
0.5	0.5	0.9162	1.36219	-0.02354	7.76007	-0.86066	8.074	-0.68479
0.4	0.6	0.9073	1.36420	-0.03076	8.56538	-0.72014	9.206	-0.8167
0.3	0.7	0.9062	1.36621	-0.03798	9.31263	-0.78314	10.145	-0.98351
0.2	0.8	0.8975	1.36722	-0.04519	10.12903	-0.48881	11.083	-1.09275
0.1	0.9	0.8887	1.36823	-0.05241	10.96613	-0.08195	12.0223	-1.18129

From table no 2, 3, 4 and 5, it is found that values of excess molar volume, are negative for entire range of compositions, which represents a decrease in the overall volume of the binary mixture. These values of excess molar volume indicate specific intermolecular force of interactions. This is further confirmed from the fact that experimental values are smaller than ideal values of binary mixtures. The experimental findings suggest that in mixtures, packing of molecules is more compact than in pure liquids.

The values of excess refractive index are negative for entire range of compositions, which represents strong intermolecular forces of interaction (table no 2 and 4). It also indicates that like nature molecules (polar-polar and non polar- non polar) are associated strongly. The values of excess refractive index are positive (table no 3 and 5) for polar and non –polar system, suggesting that their molecular associations are weak.

From the values of experimental molar refraction and calculated molar

refraction, it is further verified that molar refraction is an additive and constitutive property.

The excess molar volume and excess refractive index values of binary mixtures show that optical (refractive index) method is more refined over volumetric method.

CONCLUSIONS

From above results and discussions, it is concluded that like nature (polar-polar and non polar- non polar) molecules are strongly associated and dislike nature (polar-non polar) molecules are weakly associated. Optical method is more accurate than volumetric method.

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